

Combination of the single-double coupled cluster and the configuration interaction methods; application to barium, lutetium and their ions.

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A version of the method of accurate calculations for few valence-electron atoms which combines linearized single-double coupled cluster method with the configuration interaction technique is presented. The use of the method is illustrated by calculations of the energy levels for Ba, Ba⁺, Lu, Lu⁺ and Lu²⁺. Good agreement with experiment is demonstrated and comparison with previous version of the method (Safronova *et al*, PRA **80**, 012516 (2009)) is made.

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I. INTRODUCTION

Many-electron atoms play an important role in studying fundamental laws of modern physics and searching for new physics beyond the standard model. They are used for measurements of parity and time invariance violation in atoms (see, e. g. reviews [1, 2]), search for space-time variation of fundamental constants (see, e. g. reviews [3, 4]), etc. Another important area of application is the construction of very accurate atomic [5] and nuclear [6] clocks. Planning and interpreting the measurements require accurate atomic calculations. The calculations are also needed to address the lack of experimental data, e.g. for such systems as superheavy elements [7, 8] and highly-charged ions [9].

For atoms with one external electron above closed-shell core the best results are achieved by the use of all-order techniques based on either different versions of the coupled-cluster method [10–12] or correlation potential (CP) method [13, 14]. For heavy atoms with several valence electrons the most accurate methods include multi-configurational Hartree-Fock method (MCHF) [15] and different versions of the configuration interaction techniques. There are also versions of the CC method adopted for two-valence-electron systems [16, 17].

Configuration interaction method combined with the many-body perturbation theory to include core-valence correlations (the CI+MBPT method [18]) turned out to be a very efficient tool for accurate calculations for many-electron atoms having two or three valence electrons (see, also [19–22]). In this method core-valence correlations are included into effective CI Hamiltonian in second order of the MBPT. Recently developed method which combines CI with the linearized single-double coupled cluster method [23] takes core-valence correlations to next level of accuracy by including certain types of the core-valence correlations to all orders. The results for two and three valence electron atoms are significantly better than in the CI+MBPT method [23, 24].

In this paper an independent version of the SD+CI method is presented. It is very similar to what was presented in Ref. [23] but also has some important differences which will be discussed in next section. We

study the use of the method using barium, lutetium and their positive ions Ba⁺, Lu⁺ and Lu²⁺ as examples. We demonstrate that the accuracy of the results for ions and neutral atoms is correlated. If the SD method works well for a single-valence electron ion then the SD+CI method should give accurate results for corresponding neutral atom. This is important observation since it is well known that the SD approximation does not work well for every atomic system with one external electron (see, e.g. [26]) and triple excitations often need to be included for better accuracy. For some atoms a good alternative to the use of single-electron SD operator is the use of the all-order correlation potential [13, 14, 27].

The results of present work for Ba are in good agreement with earlier calculations of Ref. [23], in spite of some differences in the implementation of the method. We confirm that the use of the SD approximation reduces the deviation of theoretical energies from the experiment by about of factor of two as compared to the CI+MBPT method in which core-valence correlations are included in second-order of MBPT. However, better accuracy for both Ba and Ba⁺ is achieved when the all-order correlation potential [13] which includes ladder diagrams [14] is used in place of the single-electron SD operator. The two-electron operator (screening of Coulomb interaction) is still included in the SD approximation. Deviation of theoretical energies from experiment are further reduced about four time for Ba⁺ and about two times for Ba.

In contrast to Ba, the SD approximation produces very accurate results simultaneously for Lu²⁺, Lu⁺ and Lu.

II. METHOD

In the single-double linearized couple cluster method (SD) the many electron wave function of an atom is written as an expansion over terms containing single and double excitations of core or valence electrons from the reference Hartree-Fock wave function into basis states above the core (see, e.g. Ref. [10]). The coefficients of the expansion are found by solving the SD equations. The SD

equations for the core have a form [10]

$$\begin{aligned}
(\epsilon_a - \epsilon_m)\rho_{ma} &= \sum_{bn} \tilde{g}_{mban}\rho_{nb} + \\
\sum_{bnr} g_{mbnr}\tilde{\rho}_{nrab} - \sum_{bcn} g_{bcn}\tilde{\rho}_{mnbc}, \\
(\epsilon_a + \epsilon_b - \epsilon_m - \epsilon_n)\rho_{mnab} &= g_{mnab} + \\
\sum_{cd} g_{cdab}\rho_{mncd} + \sum_{rs} g_{mnrs}\rho_{rsab} + \\
\sum_r g_{mnrb}\rho_{ra} - \sum_c g_{cnab}\rho_{mc} + \sum_{rc} \tilde{g}_{cnrb}\tilde{\rho}_{mrac} + \\
\sum_r g_{nmra}\rho_{rb} - \sum_c g_{cmba}\rho_{nc} + \sum_{rc} \tilde{g}_{cmra}\tilde{\rho}_{nrbc}
\end{aligned} \quad (1)$$

Here parameters g are Coulomb integrals

$$g_{mnab} = \int \int \psi_m^\dagger(r_1)\psi_n^\dagger(r_2)\frac{e^2}{r_{12}}\psi_a(r_1)\psi_b(r_2)d\mathbf{r}_1d\mathbf{r}_2,$$

parameters ϵ are the single-electron Hartree-Fock energies. Coefficients ρ_{ma} and ρ_{mnab} are the expansion coefficients which are to be found by solving the equations iteratively starting from

$$\begin{aligned}
\rho_{mnij} &= \frac{g_{mnij}}{\epsilon_i + \epsilon_j - \epsilon_m - \epsilon_n}, \\
\rho_{ma} &= 0.
\end{aligned} \quad (2)$$

The tilde above g or ρ means the sum of direct and exchange terms, e.g.

$$\tilde{\rho}_{nrbc} = \rho_{nrbc} - \rho_{nrbc}.$$

Indexes a, b, c numerate states in atomic core, indexes m, n, r, s numerate states above the core, indexes i, j numerate any states.

The correction to the energy of the core

$$\delta E_C = \frac{1}{2} \sum_{mnab} g_{abmn}\tilde{\rho}_{nmab} \quad (3)$$

is used to control the convergence.

In the case of single electron above closed-shell core the SD equations for a particular valence state v can be obtained from (1) by replacing index a by v and replacing ϵ_a by $\epsilon_v + \delta\epsilon_v$ where

$$\delta\epsilon_v = \sum_{mab} g_{abvm}\tilde{\rho}_{mvab} + \sum_{mnb} g_{vbm}\tilde{\rho}_{mnvb} \quad (4)$$

is a correction to the energy of the valence electron. The SD equations are solved iteratively first for the core and than for as many valence states v as needed.

In the case of more than one valence electron above closed-shell core interaction between valence electrons needs to be included. This can be done with the use of the configuration interaction (CI) technique. To combine the CI technique with the SD method one needs to modify the SD equations for valence states. The SD

equations for the core (1) remain the same. To see why and how the equations should be modified it is instructive to consider an example – the use of the CI technique for an atom with one external electron above closed shells. The result of the CI calculations for such system must be equivalent to the SD calculations and the resulting energy of the calculated state should be very close to those given by Eq. (4). However, no valence state is treated in the CI approach as an initial approximation. Instead, all single electron states of the same symmetry are treated as a basis and the wave function of the valence electron is presented as an expansion

$$\psi_v = \sum_n c_n \psi_n. \quad (5)$$

Here ψ_n are single-electron basis states lying above the core, expansion coefficients c_n and the energy of the valence state v are to be found via matrix diagonalization. The SD equations should be run for every basis state ψ_n in the expansion. However, the energy parameter in all these SD equations must be the same and close to the energy of the state which is to be found. If the lowest state of the given symmetry is to be found then the natural choice is to use the Hartree-Fock energy of the lowest valence basis state.

Another modification comes from the need to exclude double counting. All terms in the SD equations which have only excitations of valence electrons must be removed since valence excitations are included in the CI calculations.

The modified SD equations for valence states have the form

$$\begin{aligned}
(\epsilon_0 - \epsilon_m)\rho_{mv} &= \sum_{bn} \tilde{g}_{mban}\rho_{nb} + \\
\sum_{bnr} g_{mbnr}\tilde{\rho}_{nrvb} - \sum_{bcn} g_{bcvn}\tilde{\rho}_{mnbc}, \\
(\epsilon_0 + \epsilon_b - \epsilon_m - \epsilon_n)\rho_{mnvb} &= g_{mnvb} + \\
\sum_{cd} g_{cdvb}\rho_{mncd} + \sum_{rs} g_{mnrs}\rho_{rsvb} - \\
\sum_c g_{cnvb}\rho_{mc} + \sum_{rc} \tilde{g}_{cnrb}\tilde{\rho}_{mrvc} + \\
\sum_r g_{nmrv}\rho_{rb} - \sum_c g_{cmbv}\rho_{nc} + \sum_{rc} \tilde{g}_{cmrv}\tilde{\rho}_{nrbc}.
\end{aligned} \quad (6)$$

These equations are obtained from (1) by replacing core index a by valence index v , removing the term $\sum_r g_{mnrb}\rho_{rv}$ which has only valence excitations, and replacing ϵ_a by ϵ_0 . The energy parameter ϵ_0 is fixed and is the same for all states in the expansion (5). Usually it is chosen to be the Hartree-Fock energy of the lowest basis state of given symmetry. Note that expression (4) is not used in the CI calculations. Instead, the energy of the valence state is found as an eigenstate of the CI matrix. This approach is very similar to one used in Ref. [25] for positron binding to atoms. It can also be used for negative ions. Neither positron nor extra electron are bound

to an atom in the Hartree-Fock approximation. Therefore, their states above the core cannot be used as initial approximation but should be used as basis states for the CI calculations.

In case of more than one external electron, the Coulomb interaction between valence electrons needs to be modified as well. Replacing in the equations for the double excitation coefficients (1) core indexes a, b by valence indexes v, w and removing terms which have only valence excitations we get the expressions for screened Coulomb integrals to be used in the CI calculations

$$\begin{aligned} q_{mnvw} = & g_{mnvw} + \sum_{cd} g_{cdvw} \rho_{mncd} - \sum_c (g_{cnvw} \rho_{mc} + g_{cmvw} \rho_{nc}) + \\ & \sum_{rc} (g_{cnrw} \tilde{\rho}_{mrvc} + g_{cmrv} \tilde{\rho}_{nrwc} + g_{cnwr} \rho_{mrvc} \\ & + g_{cmvr} \rho_{nrwc} - g_{cmwr} \rho_{nrvc} - g_{cnvr} \rho_{mrwc}) \end{aligned} \quad (7)$$

The effective CI Hamiltonian can be written as a sum of one and two electron parts

$$\hat{H}^{\text{CI}} = \sum_i^{N_v} \hat{h}_1(r_i) + \sum_{i < j}^{N_v} \hat{h}_2(r_i, r_j). \quad (8)$$

Here N_v is the number of valence electrons. The single electron part is given by

$$\hat{h}_1 = \alpha \mathbf{p} + (\beta - 1)mc^2 + V_{\text{core}} + \hat{\Sigma}_1, \quad (9)$$

where α and β are Dirac matrixes, V_{core} is the self-consistent potential of the atomic core (including nuclear part), $\hat{\Sigma}_1$ is the single-electron correlation operator responsible for the correlation interaction of a valence electron with the core. Its matrix elements are obtained from (6) and can be written as

$$\langle v | \hat{\Sigma}_1 | m \rangle = (\epsilon_0 - \epsilon_m) \rho_{mv}. \quad (10)$$

The two-electron part \hat{h}_2 of the CI Hamiltonian (8) is the sum of the Coulomb interaction and the two-electron correlation operator $\hat{\Sigma}_2$. Matrix elements of \hat{h}_2 in the SD approximation are given by (7).

The notation $\hat{\Sigma}$ for the operator of the core-valence correlations was introduced in Ref. [18] in the framework of the CI method combined with the many-body perturbation theory (MBPT). In this and following works [19–22] the $\hat{\Sigma}_1$ and $\hat{\Sigma}_2$ operators were calculated in the lowest second-order of the MBPT. This corresponds to substituting the initial approximation (2) into (6) and (7) without iterating the SD equations (1,6). Thus, present work further advances the method by including higher-order correlations. This leads to significant improvement in the accuracy of the calculations for many atomic systems.

The SD+CI method was first developed in Ref. [23]. Its implementation in present work is independent and slightly different. Most of the difference is in energy denominators. Energy denominators in equations (6) and

(7) are hidden in the expressions for the excitation coefficients ρ . In corresponding expressions of Ref. [23] (see Eq.(22-24) in [23]) the energy denominators are shown explicitly and they are different from what can be found in (6) and (7). Energy denominator of every term containing valence state v is corrected in [23] by the energy difference $\tilde{\epsilon}_v - \epsilon_v$, where ϵ_v is the Hartree-Fock energy of the valence state v and $\tilde{\epsilon}_v$ is an external parameter. It can be chosen to be the energy of the lowest state of given symmetry or it can be used as a fitting parameter. Let us consider in more detail why different energy denominators may appear.

Moving core excitations into valence space leads to the following second-order corrections to the matrix elements of the CI Hamiltonian [18]

$$\Delta H_{IJ}^{\text{CI}} = \sum_M \frac{\langle I | U | M \rangle \langle M | U | J \rangle}{E - E_M}, \quad (11)$$

where U is residual Coulomb interaction, $|I\rangle$ and $|J\rangle$ are many-electron states in the valence space, states $|M\rangle$ are many electron states with excitations from the core, E_M is the many-electron energy of the state $|M\rangle$, E is the energy of the state to be found in the calculations. Expression (12) corresponds to the Brillouin-Wigner (BW) version of the MBPT. The alternative is to use the Rayleigh-Schrödinger (RS) MBPT in which Eq. (12) transfers to

$$\Delta H_{IJ}^{\text{CI}} = \sum_M \frac{\langle I | U | M \rangle \langle M | U | J \rangle}{E_I - E_M}. \quad (12)$$

There are two reasons to use the BW MBPT rather than the RS one. First, the CI matrix is not symmetric in the RS approach, $H_{IJ}^{\text{CI}} \neq H_{JI}^{\text{CI}}$. Second, energy denominator $E_I - E_M$ for highly excited state $|I\rangle$ may accidentally become very small leading to unphysical enhancement of otherwise small contribution.

The downside of the use of the BW version of the MBPT is that there is no exact solution to the problem of reducing the many-electron expression (12) to single- and two-electron operators $\hat{\Sigma}_1$ and $\hat{\Sigma}_2$. Thus different approximations can be used.

One can see from (12) that the core-valence correlation operator $\hat{\Sigma}$ is the energy-dependent operator which should be calculated at the energy close to the energy of the state of interest. The $\tilde{\epsilon}_v - \epsilon_v$ corrections to the energy denominators used in Ref. [23] were introduced to ensure correct dependence of the $\hat{\Sigma}$ operator on the energy (see also [28]). This might be important for highly excited states. For low lying states which are always of the most interest the corrections are less important and can be neglected.

A. Basis states

A complete set of single-electron states is needed for solving the SD equations (1,6) and for construction of the

many-electron states for the CI calculations. We use the same B-spline technique [29] for both purposes. Forty B-spline states of the order of nine are calculated in a box of radius $40 a_B$ in each partial wave up to $l_{\max} = 6$. All of them are used for calculating terms in the SD equations indexes n, m, r, s in (1,6,7,10)). The SD equation for valence states are solved for few (three of four) states above the core in each partial wave up to $l_{\max} = 3$. The second-order correlation potential Σ is used for higher states. Fourteen states above the core in each partial wave up to $l_{\max} = 4$ are used in the CI calculations. With this choice of the parameters the basis is sufficiently saturated.

B. Breit and QED corrections

Breit and quantum electrodynamic (QED) corrections are not very important for barium and lutetium. We include them however to be sure that remaining deviation of the calculated energies from experiment is mostly due to higher-order correlations. We do this in the same way as in our previous works (see, e.g. [27, 30]).

We treat Breit interaction in zero energy transfer approximation. The Breit Hamiltonian includes magnetic interaction and retardation:

$$\hat{H}^B = -\frac{\boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2 + (\boldsymbol{\alpha}_1 \cdot \mathbf{n})(\boldsymbol{\alpha}_2 \cdot \mathbf{n})}{2r}. \quad (13)$$

Here $\mathbf{r} = \mathbf{n}r$, r is the distance between electrons, and $\boldsymbol{\alpha}$ is the Dirac matrix.

Breit interaction is included in the self-consistent Hartree-Fock procedure. Thus the effect of Breit interaction on self consistent atomic potential is included. This effect, which is often called the relaxation effect, is still linear in Breit but non-linear in Coulomb interaction. Its inclusion leads to more accurate results than treating Breit interaction perturbatively.

To include the QED corrections we use the radiative potential approach developed in Ref. [31]. This radiative potential has the form

$$V_{\text{rad}}(r) = V_U(r) + V_g(r) + V_e(r), \quad (14)$$

where V_U is the Uehling potential, V_g is the potential arising from the magnetic formfactor, and V_e is the potential arising from the electric formfactor. The V_U and V_e terms can be considered as additions to nuclear potential while inclusion of V_g leads to some modification of the Dirac equation (see Ref. [31] for details).

III. RESULTS

Performing calculations in the V^{N-2} approximation for Ba and V^{N-3} approximation for Lu we have pairs of atomic systems with similar electron structure. Ba has electron structure similar to Lu^+ and Ba^+ is similar to Lu^{2+} . It is natural to expect some similarities in the

TABLE I: Removal energies (cm^{-1}) of the lowest s, p, d states of Ba^+ in SD+CI and CP+CI approximations. $\Delta = E_{\text{theor}} - E_{\text{expt}}$.

State	SD+CI	Δ	CP+CI	Δ	Expt. ^b
$6s_{1/2}$	81210	524	80719	33	80686
$5d_{3/2}$	76341	529	75969	157	75812
$5d_{5/2}$	75474	463	75108	97	75011
$6p_{1/2}$	60710	286	60512	88	60424
$6p_{3/2}$	58980	246	58794	60	58734

^aRef. [32].

results. It turns out however that barium and lutetium are sufficiently different so that best results are achieved with slightly different procedures. We will therefore discuss them separately.

A. Barium and its positive ion

Table I presents results of calculations of the energy levels of Ba^+ . As one can see the accuracy of the SD approximation for the ion is on the level 0.5 - 0.7%. Significantly better accuracy can be achieved if the all-order correlation potential [13, 14] is used [27]. Corresponding numbers are presented in Table I under the header "CP+CI". Note that these numbers are slightly different from those presented in Ref. [27]. The difference is due to the fact that in present work the energies were obtained as a result of matrix diagonalization while in Ref. [27] they were found by solving single-electron equations for Brueckner orbitals.

Similar improvement in accuracy of the calculations can be achieved for neutral barium if single-electron SD matrix elements (10) are replaced by the matrix elements of the all-order correlation potential as in Ref. [27].

The results for neutral barium are presented in Table II. The results of previous calculations in the SD+CI approximation [23] are also presented for comparison. As one can see, in spite of some difference in the methods (see discussion of energy denominators in section II), the results of both SD+CI calculations are very close to each other. It was pointed out in Ref. [23] that the deviation of the calculated energies from experiment in the SD+CI calculations is about two times smaller than in the CI+MBPT calculations. This is the effect of selected higher-order core valence correlations included in the SD+CI method but not in the CI+MBPT method. Which higher-order correlations play the most important role varies from atom to atom. The SD approximation is not always the best choice. It turns out that for barium better results are achieved when single-electron SD matrix elements (10) are replaced by the matrix elements of the all-order correlation potential, while screened Coulomb integrals are kept the same (see Eq. (7)). Corresponding results are presented in Table II in the CP+CI column. As one can see, the difference with

TABLE II: Excitation energies (cm^{-1}) of the lowest states of Ba in SD+CI and CP+CI approximations; $\Delta = E_{\text{theor}} - E_{\text{expt}}$.

State	J	Ref. [23]		This work				Expt. ^a
		SD+CI	Δ	SD+CI	Δ	CP+CI	Δ	
$6s^2 \ ^1S$	0	0		0		0		0
$6s5d \ ^3D$	1	9249	216	8882	-151	8936	-97	9033
	2	9441	225	9132	-84	9187	71	9216
	3	9840	243	9505	-92	9560	-37	9597
$6s5d \ ^1D$	2	11721	326	11471	76	11508	113	11395
$6s6p \ ^3P^o$	0	12556	290	12541	275	12325	59	12266
	1	12919	282	12898	261	12679	42	12637
	2	13819	304	13796	281	13568	53	13515
$6s6p \ ^1P^o$	1	18292	232	18173	113	17973	-87	18060
$5d^2 \ ^3F$	2			20722	-212	20850	-84	20934
	3			20956	-294	21080	-170	21250
	4			21462	-162	21584	-40	21624
	4			22154	89	22006	-59	22065
$5d6p \ ^3F^o$	3			23050	103	22916	-31	22947
	4			23912	155	23768	11	23757
	4			22931	-131	23062	0	23062
$5d^2 \ ^1D$	2			23237	163	23035	-39	23074
$5d6p \ ^1D^o$	2			22729	-480	22862	-212	23209
$5d^2 \ ^3P$	0			22877	-603	23018	-462	23480
	1			23663	255	23794	-124	23918
	2			24266	74	24044	-148	24192
$5d6p \ ^3D^o$	1			24635	103	24410	-122	24532
	2			25110	130	24885	-95	24980
	3			25721	79	25528	-114	25642
$5d6p \ ^3P^o$	0			25789	85	25600	-104	25704
	1			26088	131	25902	-55	25957
	2			26425	265	26135	-25	26160

^aRef. [32].

the experimental energies is further reduced by about two times.

The accuracy of present calculations for barium is better than in previous calculations with the use of the CI+MBPT method [19, 33, 34]. This is in spite of the fact that present calculations are pure *ab initio* ones while in earlier calculations rescaling of the second-order correlation operator $\hat{\Sigma}$ was used to fit the energies of the lowest states.

B. Lutetium and its ions

The results for energy levels of Lu^{2+} are presented in Table III. There are two sets of the SD results. One (called SD) corresponds to the standard SD method for atoms with one external electron in which the SD equations are iterated for a specific valence state and correction to the energy is calculated using (4). Another set (called SD+CI) is based on the CI method. Hartree-Fock valence states are treated as a basis (as in Eq. (5)) and the energy of the valence state is found as an eigenstate of the CI Hamiltonian. This two approaches are almost

TABLE III: Removal energies (cm^{-1}) of the lowest s, p, d states of Lu^{2+} in SD and SD+CI approximations. $\Delta = E_{\text{theor}} - E_{\text{expt}}$.

State	SD	Δ	SD+CI	Δ	Expt. ^a
$6s_{1/2}$	169705	691	169723	709	169014
$5d_{3/2}$	163324	18	163241	-65	163306
$5d_{5/2}$	160304	-62	160204	-162	160366
$6p_{1/2}$	130956	343	131017	404	130613
$6p_{3/2}$	124558	249	124587	278	124309

^aRef. [32].

equivalent. Some small difference in results is mostly due to the fact that equations (6) used in the CI calculations are iterated with the fixed energy parameter ϵ_0 while energy of the valence state (4) in the standard SD method changes on every iteration. Other factor which can make minor contribution to the difference is incompleteness of the basis in the expansion (5) and the fact that the SD equations (6) are iterated only for few first basis states in the expansion. In the end the difference between SD and SD+CI results is very small. The difference of theses result and experiment is also small. It is on the level 0.4% or better. This reflects general trend for isoelectronic sequences of alkali atoms. For example, the SD approximation gives poor accuracy for cesium [26], better accuracy for Ba^+ (see Table I) and even better accuracy for Lu^{2+} . In contrast to Ba^+ , using the correlation potential method does not lead to improvement in accuracy. Therefore we limit further calculations to the SD+CI method.

Tables IV and V show the results of the SD+CI calculations for the energy levels of Lu^+ and Lu. The results of previous similar calculations for Lu are also shown for comparison.

IV. CONCLUSION

A version of the method of calculations for many-electron atoms which combines configuration interaction with the single-double linearized coupled cluster approach is presented. This version is simpler than previous one but gives results on the same level of accuracy. The accuracy is better than in the widely used CI+MBPT method. It can be further improved with a different choice of the single-electron correlation operator $\hat{\Sigma}$. The best choice for barium is the all-order correlation potential which was widely used before for the systems with one external electron above closed shells. It is demonstrated that the accuracy of calculation for neutral atoms and positive ions of these atoms is correlated. Therefore, one can choose an adequate approximation for the ions first before proceeding to neutral atoms. This is very convenient since calculations for ions take much less computer resources. In the end, we have another method which can be widely used for accurate calculations in many

TABLE IV: Excitation energies (cm^{-1}) of the lowest states of Lu^+ in SD+CI; $\Delta = E_{\text{theor}} - E_{\text{expt}}$.

State	J	SD+CI	Δ	Expt. ^a
$6s^2$ 1S	0	0	0	0
$6s5d$ 3D	1	11948	152	11796
	2	12695	260	12435
	3	14473	274	14199
$6s5d$ 1D	2	17892	560	17332
$6s6p$ $^3P^o$	0	27657	393	27264
	1	28891	388	28503
	2	32918	465	32453
$6s6p$ $^1P^o$	1	18292	232	18060
$5d^2$ 3F	2	29751	345	29406
	3	31238	349	30889
	4	32985	482	32503
$5d^2$ 3P	0	35673	21	35652
	1	36574	17	36557
	2	39202	628	38574
$5d^2$ 1D	2	36563	465	36098
$5d6p$ $^3F^o$	2	41789	565	41224
	3	45575	657	44918
	4	49304	739	48536
$5d6p$ $^1D^o$	2	46149	691	45458
$5d6p$ $^3D^o$	1	46015	483	45532
	2	47474	570	46904
	3	49359	626	48733
$5d6p$ $^3P^o$	0	50505	542	49963
	1	50616	567	50049
	2	51884	683	51201

^aRef. [32].

atomic systems.

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TABLE V: Excitation energies (cm^{-1}) of the lowest states of Lu in SD+CI approximation; comparison with previous work and experiment. $\Delta = E_{\text{theor}} - E_{\text{expt.}}$

State	J	Ref. [35]		This work		Expt. ^a
		Energy	Δ	Energy	Δ	
$5d6s^2$	2D	3/2	0	0		0
		5/2	2014	2123	129	1994
$6s^26p$	$^2P^o$	1/2	3910	3975	-161	4136
		3/2	7228	7367	-109	7476
$5d6s6p$	$^4F^o$	3/2	17723	17502	75	17427
		5/2	18789	18652	147	18505
		7/2	20731	20596	163	20433
		9/2	22911	22786	177	22609
$5d^26s$	4F	3/2	19182	18662	-189	18851
		5/2	19737	19248	-155	19403
		7/2	20578	20095	-152	20247
		9/2	21591	21159	-83	21242
$5d6s6p$	$^4D^o$	1/2	20995	20795	33	20762
		3/2	21448	21284	89	21195
		5/2	22504	22352	130	22222
		7/2	23795	23665	141	23524
$5d6s6p$	$^2D^o$	3/2	22376	22534	410	22125
		5/2	21735	21775	313	21462
$5d^26s$	4P	5/2	23242	23084	282	22802
		1/2	21860	21803	331	21472
		3/2	22849	22671	203	22468
$5d6s6p$	$^4P^o$	1/2	24520	24262	153	24109
		3/2	24786	24563	255	24308
		5/2	25774	25524	332	25192
$6s^27s$	2S	1/2		25408	890	24126
$5d^26s$	2D	3/2	25015	25128	-390	24518
		5/2		25162	-549	24711

^aRef. [32].

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